



NORTH-HOLLAND

Numerical Solutions for Large Sparse Quadratic Eigenvalue Problems

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ABSTRACT

We study the quadratic eigenvalue problem $(A + \lambda B + \lambda^2 C)x = 0$, where A , B , and C are symmetric real $n \times n$ matrices, and A , C are positive definite. We propose an efficient numerical algorithm to compute a few of the smallest positive eigenvalues of the problem and their associated eigenvectors. The new algorithm includes two parts. The first part gives iterative methods which can be used to compute the smallest positive eigenvalue. We develop a globally linearly convergent basic iteration and two locally quadratically convergent iterations. The second part uses the nonequivalence deflation technique. This technique allows us to transform the original problem to a new problem with different A , B , and C . The new problem has the same eigenvalues as the old problem except that the smallest positive eigenvalue of the old problem is replaced by zero. Therefore, the second smallest positive eigenvalue of the old problem becomes the smallest positive one for the new problem. Then the above proposed iterative methods can be applied again to find the second smallest positive eigenvalue. Proceeding in this way, we can find out the 3rd, 4th, ... smallest positive eigenvalues. Our algorithm utilizes the symmetry and positivity of the given matrices, and avoids computing the undesired complex conjugate eigenvalues. Under some mild conditions, is efficient and reliable. The above process can also be used to find a few of the largest negative eigenvalues.

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1. INTRODUCTION

Given symmetric real $n \times n$ matrices A , B , and C with A and C positive definite. We are concerned with the numerical solutions for the quadratic eigenvalue problem of the form

$$F(\lambda)x \equiv (A + \lambda B + \lambda^2 C)x = 0. \quad (1.1)$$

Hereafter we shall refer to the problem (1.1) with A positive definite as (DP).

Problems (DP) arise in the analysis of geometrical nonlinear buckling structures with finite element methods [1, 3, 4, 6]. In these cases the matrices A , B , and C under considerations are large and banded. The real eigenvalue λ of (DP) is usually the factor of safety for the applied external force in the buckling structure, and the associated eigenvector x is the buckling mode shape. Since the higher buckling modes only describe the behavior of a structure that would have buckled under a lighter load and rarely have engineering meaning, it is usually the case that only a few of the smallest real eigenvalues in modulus are important. If the load is thought of as being applied in one direction, then only either positive or negative eigenvalues are significant. For the convenience of discussion, we hence focus our attention on developing an efficient algorithm to compute a few of the smallest positive eigenvalues of (DP) and their associated eigenvectors.

Letting $\mu = 1/\lambda$, by an intuitive consideration the quadratic eigenvalue problem (DP) can be transformed to an enlarged linear eigenvalue problem

$$\begin{bmatrix} -C & O \\ O & A \end{bmatrix} \begin{bmatrix} \lambda x \\ x \end{bmatrix} = \mu \begin{bmatrix} B & A \\ A & O \end{bmatrix} \begin{bmatrix} \lambda x \\ x \end{bmatrix}. \quad (1.2)$$

Since both enlarged $2n \times 2n$ matrices in (1.2) are indefinite, the eigenvalues μ can be complex. Some well-known algorithms such as subspace iteration [14], the Arnoldi method with Chebychev acceleration [24, 25], and the unsymmetric Lanczos method [7, 21] can be applied on the matrix

$$\begin{bmatrix} B & A \\ A & O \end{bmatrix}^{-1} \begin{bmatrix} -C & O \\ O & A \end{bmatrix}$$

to solve the eigenvalue problem (1.2). In practice, all the above methods always converge faster to the extreme eigenvalues, i.e. the eigenvalues which

lie on the boundary of the spectrum. If our desired real eigenvalues are not the extreme values, then these methods are not suitable for solving the problem (1.2). Besides, no elegant theory of convergence analysis has been developed. From practical point of view, the shift-invert technique [10] can be considered to solve the problem (1.2). This technique is reliable when the matrix on the right-hand side of (1.2) are positive semidefinite. In 1990, Parlett and Chen [20] formally used the symmetric Lanczos method by utilizing the shift-invert technique to solve the symmetric indefinite pencil as in (1.2). Since both matrices of (1.2) are indefinite, the shift-invert technique has its dangers. It is pointed out in [20] that undetectable growth of Lanczos vectors in certain directions and breakdown of the algorithm are problems that remain unsolved.

The quadratic eigenvalue problem has been studied for some time. Lancaster et al. [11, 17, 18] provided a good theoretical treatment of the subject and explored the application to vibrating systems. By numerical algorithms, Kublanovskaja [16], Ruhe [23], and Peters and Wilkinson [22] presented some Newton-type algorithms for the calculation of eigenvalues of general λ -matrix polynomials. All these methods are only locally quadratically convergent. There is no guarantee of convergence to the smallest positive eigenvalue even if a zero is chosen as initial value. Besides, the symmetry and positivity property of the matrices in (DP) are not utilized. Some deflation strategies proposed by Ruhe [23] for finding the second smallest positive eigenvalue require complex arithmetic calculations. In 1981 Davis [8] proposed as efficient numerical algorithm for the calculating the solvent $X \in \mathbb{C}^{n \times n}$ for the quadratic matrix equation

$$F(X) \equiv A + BX + CX^2 = 0.$$

This equation is very closely related to the problem of finding scalar λ and nonzero vector x such that (1.1) holds.

For a given real λ , we now consider the linear symmetric eigenvalue problem

$$\beta(\lambda) Ax(\lambda) = -(B + \lambda C)x(\lambda). \quad (1.3)$$

Since A is symmetric positive definite and $-(B + \lambda C)$ is real symmetric, the eigenvalues of (1.3) are all real and can be labeled as

$$\beta_1(\lambda) \geq \beta_2(\lambda) \geq \cdots \geq \beta_n(\lambda). \quad (1.4)$$

We call the curve defined by the function $\beta_i(\lambda)$, $i = 1, \dots, n$, the i th eigenvalue curve. It can be proven that these functions are all strictly decreasing. Therefore, to find the smallest positive eigenvalue of (DP) it is sufficient to find the smallest fixed point of the function $1/\beta_1(\lambda)$ for $\lambda > 0$. Three iteration methods given in Section 2 can be used to compute this fixed point.

To obtain the second smallest positive eigenvalue, we develop a so-called nonequivalence transformation (see Section 3 for details). This allows us to transform the original problem to a new problem in which the matrix corresponding to the A -term is positive semidefinite. Moreover, the new problem has the same eigenvalues as the old problem except that the smallest positive eigenvalue of the old problem is replaced by zero. Now, the second smallest positive eigenvalue of the old problem becomes the smallest positive eigenvalue of the new, transformed problem. Hence, the three iteration methods given in Section 2 can be applied again to compute this eigenvalue. Proceeding in this way, we can obtain the 3rd, 4th, \dots smallest positive eigenvalues of (DP) when these desired eigenvalues satisfy some mild restrictions (see comments in Algorithm 5.1). We remark that when A is positive semidefinite, then the labeled eigenvalue curves as in (1.4) are allowed to be $\pm\infty$. We will show that the finite eigenvalue curves are strictly decreasing and analyze their asymptotic behavior.

We organize this paper as follows. In Section 2, we give a basic iteration with global linear convergence rate, and the tangent and Newton iterations with local quadratic convergence rate, for finding the current smallest positive eigenvalue. In Section 3, we develop the nonequivalence transformation for the quadratic eigenvalue problem. We give the relations of eigenvalues and the associated eigenvectors between the original and the new transformed problems. In Section 4, we give some properties of the eigenvalue curves $\beta(\lambda)$ of (1.3) for the more general case that A is positive semidefinite. In Section 5, we use the iteration methods of Section 2 and the results of Sections 3 and 4 to develop an efficient algorithm for finding a few of the smallest positive eigenvalues and their associated eigenvectors. Some numerical results are also given. Finally, the conclusions are given in Section 6.

2. ITERATIVE METHODS

In this section we propose three iterative methods for finding the smallest positive eigenvalue of (DP). Since A is positive definite, by a well-known result of [15] the eigenvalue curve $\beta(\lambda)$ in (1.3) is differentiable at λ except at a finite number of exceptional points and the derivative of $\beta(\lambda)$ is equal to

$-x^T(\lambda)Cx(\lambda)$. Because of the positivity of the matrix C the eigenvalue curves $\beta_j(\lambda)$, for $j = 1, \dots, n$, are strictly decreasing. It follows that the smallest positive eigenvalue of (DP) is the smallest positive fixed point of the function $1/\beta_1(\lambda)$. Let λ_* denote the smallest positive eigenvalue of (DP). Then λ_* is the fixed point of the function $1/\beta_1(\lambda)$. In the following we give three iterative methods for finding λ_* .

BASIC ITERATIVE METHOD.

1. Given an initial guess $\lambda_0 \geq 0$. Let $p = 0$.
Repeat:
2. Call the symmetric Lanczos algorithm [19] to compute the eigenpair $(\beta_1(\lambda_p), x_1(\lambda_p))$ of the generalized eigenvalue problem

$$\beta(\lambda_p)Ax(\lambda_p) = -(B + \lambda_p C)x(\lambda_p).$$
3. Let $\lambda_{p+1} = 1/\beta_1(\lambda_p)$.
4. If $|\lambda_{p+1} - \lambda_p| \leq \text{Tolerance}$, then
 set $\lambda_* = \lambda_{p+1}$ and stop,
 else $p := p + 1$, $\lambda_p := \lambda_{p+1}$, goto Repeat.

THEOREM 2.1. *In the basic iterative method, if $\beta_1(0) > 0$, then the sequence $\{\lambda_p\}$ converges to λ_* as $p \rightarrow \infty$. Moreover, if $(1/\beta_1)'(\lambda_*) < 1$, then $\{\lambda_p\}$ is linearly convergent.*

Proof. Since $\beta_1(0) > 0$ and $\beta_1(\lambda)$ is strictly decreasing, by induction we see that the sequence $\{\lambda_p\}$ is increasing and satisfies $0 < \lambda_p \leq \lambda_*$. Hence the sequence $\{\lambda_p\}$ converges. Suppose that λ_p converges to $\mu_* < \lambda_*$, as $p \rightarrow \infty$. Since $\lambda_{p+1} = 1/\beta_1(\lambda_p)$, taking $p \rightarrow \infty$ in both sides, we get $\mu_* = 1/\beta_1(\mu_*)$. Thus, μ_* is the smallest positive fixed point of $1/\beta_1(\lambda)$. But $\mu_* < \lambda_*$, so this is a contradiction. Therefore $\{\lambda_p\} \rightarrow \lambda_*$ as $p \rightarrow \infty$.

For linear convergence, we note that

$$\begin{aligned} \frac{\lambda_{p+1} - \lambda_*}{\lambda_p - \lambda_*} &= \frac{1/\beta_1(\lambda_p) - 1/\beta_1(\lambda_*)}{\lambda_p - \lambda_*} \\ &= \frac{\beta_1(\lambda_*) - \beta_1(\lambda_p)}{\beta_1(\lambda_p)\beta_1(\lambda_*)(\lambda_p - \lambda_*)} \\ &= \frac{-\beta_1'(\xi_p)}{\beta_1(\lambda_p)\beta_1(\lambda_*)} \end{aligned} \tag{2.1}$$

for some ξ_p between λ_p and λ_* , by the mean-value theorem. Since the quantity on the right-hand side of (2.1) tends to $(1/\beta_1)'(\lambda_*)$ as $p \rightarrow \infty$,

which is less than one, the linear convergence for the basic iteration method follows. ■

The basic iterative method ensures that the iteration always converges with linear convergence rate. In order to accelerate the convergence, we develop the tangent and Newton iterative methods.

Tangent Iterative Method.

1. Given an initial guess $\lambda_0 \geq 0$. Let $p = 0$.
Repeat:
2. Call the symmetric Lanczos algorithm [19] to compute the eigenpair $(\beta_1(\lambda_p), x_1(\lambda_p))$ of the generalized eigenvalue problem

$$\beta(\lambda_p) Ax(\lambda_p) = -(B + \lambda_p C)x(\lambda_p).$$

3. Compute

$$b(\lambda_p) = \beta_1(\lambda_p) - \beta'_1(\lambda_p)\lambda_p \text{ and}$$

$$c(\lambda_p) = b(\lambda_p)^2 + 4\beta'_1(\lambda_p),$$

where

$$\beta'_1(\lambda_p) := -x_1(\lambda_p)^T C x_1(\lambda_p).$$

4. If $c(\lambda_p) \geq 0$, then

$$\text{compute } \lambda_{p+1} = \left\{ -b(\lambda_p) + [\text{sgn } b(\lambda_p)] \sqrt{c(\lambda_p)} \right\} / 2\beta'_1(\lambda_p),$$

else $\lambda_{p+1} = 1/\beta_1(\lambda_p)$ (basic iteration).

5. If $|\lambda_{p+1} - \lambda_p| \leq \text{Tolerance}$, then

$$\text{set } \lambda_* := \lambda_{p+1} \text{ and stop,}$$

else $p := p + 1$, $\lambda_p := \lambda_{p+1}$, goto Repeat.

The geometrical meaning of the tangent iterative method is that we want to compute the intersection points of the tangent of the curve $\beta_1(\lambda)$ at the point $(\lambda_p, \beta_1(\lambda_p))$ and on the hyperbola $y = 1/\lambda$. This is equivalent to solving the system of equations

$$y - \beta_1(\lambda_p) = \beta'_1(\lambda_p)(\lambda - \lambda_p),$$

$$y = 1/\lambda.$$

Hence we take the next iterate λ_{p+1} as the first coordinate of the intersection point which is closer to the y -axis.

THEOREM 2.2. *If the condition $c(\lambda_p) \geq 0$ holds for all p in step 4 of the tangent iteration and the iteration converges, then it converges quadratically.*

Proof. Let

$$g(\lambda) = \frac{-b(\lambda) + [\operatorname{sgn} b(\lambda)]\sqrt{c(\lambda)}}{2\beta'_1(\lambda)}, \quad (2.2)$$

where $b(\lambda) = \beta_1(\lambda) - \beta'_1(\lambda)\lambda$ and $c(\lambda) = b(\lambda)^2 + 4\beta'_1(\lambda)$.

We can write the tangent iteration as $\lambda_{p+1} = g(\lambda_p)$. To prove that the tangent iteration converges quadratically is equivalent to showing that if α is a fixed point of $g(\lambda)$ then $g'(\alpha) = 0$. From (2.2) the numerator of $g'(\alpha)$ becomes

$$\begin{aligned} h \equiv & -2\beta'_1(\alpha) \frac{b'(\alpha) - [\operatorname{sgn} b(\alpha)][2b(\alpha)b'(\alpha) + 4\beta''_1(\alpha)]}{2\sqrt{b^2(\alpha) + 4\beta'_1(\alpha)}} \\ & + 2\beta''_1(\alpha) \left\{ b(\alpha) - [\operatorname{sgn} b(\alpha)]\sqrt{b^2(\alpha) + 4\beta'_1(\alpha)} \right\}. \end{aligned} \quad (2.3)$$

Since $g(\alpha) = \alpha$, we have

$$b(\alpha) - [\operatorname{sgn} b(\alpha)]\sqrt{b^2(\alpha) + 4\beta'_1(\alpha)} = -2\alpha\beta'_1(\alpha). \quad (2.4)$$

Substituting $b(\alpha) = \beta_1(\alpha) - \beta'_1(\alpha)\alpha$ in (2.4), we get

$$4\beta'_1(\alpha)[\alpha\beta(\alpha) - 1] = 0. \quad (2.5)$$

Hence from (2.3) and (2.4) we obtain

$$\begin{aligned} h &= -2\beta'_1(\alpha) \left(b'(\alpha) - \frac{b(\alpha)b'(\alpha) + 2\beta''_1(\alpha)}{b(\alpha) + 2\alpha\beta'_1(\alpha)} \right) - 4\alpha\beta'_1(\alpha)\beta''_1(\alpha) \\ &= \frac{2\beta'_1(\alpha)}{b(\alpha) + 2\alpha\beta'_1(\alpha)} [b(\alpha)b'(\alpha) + 2\beta''_1(\alpha) - b(\alpha)b'(\alpha) \\ &\quad - 2\alpha b(\alpha)\beta'_1(\alpha) - 4\alpha^2\beta'_1(\alpha)\beta''_1(\alpha) \\ &\quad - 2\alpha b(\alpha)\beta''_1(\alpha)]. \end{aligned} \quad (2.6)$$

Substituting $b'(\alpha) = -\alpha\beta_1''(\alpha)$ in (2.6), we then have

$$h = -4\beta_1'(\alpha)\beta_1''(\alpha)\frac{\beta_1'(\alpha)\alpha^2 + b(\alpha)\alpha - 1}{b(\alpha) + 2\alpha\beta_1'(\alpha)}. \quad (2.7)$$

Substituting $b(\alpha) = \beta_1(\alpha) - \beta_1'(\alpha)\alpha$ again in (2.7) and using (2.5), it follows that $h = 0$ and the theorem follows. ■

We now consider the function $f(\lambda) = 1/\beta_1(\lambda) - \lambda$. The smallest positive eigenvalue λ_* of (DP) is the smallest positive root of $f(\lambda)$. Since $f(0) = 1/\beta_1(0) > 0$ and $f'(\lambda)$ exists almost everywhere, we can apply Newton's method to $f(\lambda)$ for finding λ_* .

NEWTON'S ITERATIVE METHOD.

1. Given an initial guess $\lambda_0 \geq 0$. Let $p = 0$.
Repeat:
2. Call the symmetric Lanczos algorithm [19] to compute the eigenpair $(\beta_1(\lambda_p), x_1(\lambda_p))$ of the generalized eigenvalue problem

$$\beta(\lambda_p)Ax(\lambda_p) = -(B + \lambda_p C)x(\lambda_p).$$

3. Let $r_p = -\beta_1'(\lambda_p)/\beta_1^2(\lambda_p) = x_1(\lambda_p)^T C x_1(\lambda_p)/\beta_1^2(\lambda_p)$
4. If $r_p < 1$, compute

$$\lambda_{p+1} = [\lambda_p \beta_1'(\lambda_p) + \beta_1(\lambda_p)] / [\beta_1^2(\lambda_p) + \beta_1'(\lambda_p)].$$

else if $r_p = 1$ and $\lambda_p = 1/\beta_1(\lambda_p)$, then stop,

$$\text{else } \lambda_{p+1} = 1/\beta_1(\lambda_p) \quad (\text{basic iteration}).$$

5. If $|\lambda_{p+1} - \lambda_p| \leq \text{Tolerance}$, then

$$\text{set } \lambda_* := \lambda_{p+1} \text{ and stop,}$$

else $p := p + 1$, $\lambda_p := \lambda_{p+1}$, goto Repeat.

Since Newton's method converges locally quadratically, r_p is controlled so that λ_p approaches the smallest positive root. That is, if $r_p < 1$ for all p and $\lambda_p \rightarrow \lambda_*$ as $p \rightarrow \infty$, then λ_p converges quadratically to λ_* .

3. NONEQUIVALENCE DEFLATION

We now start with the original quadratic eigenvalue problem $F(\lambda)x = 0$ in (1.1) with A and C positive definite, i.e., the problem (DP). From the positivity of C it is clearly seen that $F(\lambda)$ has $2n$ finite eigenvalues, i.e., $F(\lambda)$ is regular in the sense that $\det F(\lambda) \neq 0$ and is of degree $2n$. A regular λ -matrix polynomial $F(\lambda)$ is said to be simple at an eigenvalue μ_j if $F(\mu_j)$ has degeneracy m_j (or rank $n - m_j$), where μ_j is a root of $\det F(\lambda)$ with multiplicity m_j . $F(\lambda)$ is called a simple λ -matrix polynomial if $F(\mu_j)$ is simple for all eigenvalues μ_j , $j = 1, \dots, 2n$ [17].

Write $A_0 := A$, $B_0 := B$, and $C_0 := C$. Let (μ_0, Y_0) be a simple eigensolution of (DP) with $\text{rank } Y_0 = m_0$, obtained by the iterative methods of Section 2, where μ_0 is the smallest positive eigenvalue of (DP) with multiplicity m_0 . We want to compute the second smallest positive eigenvalue of (DP). The following nonequivalence deflation allows us to transform the original problem to a new problem with the same eigenvalues except that μ_0 is replaced by zero. Therefore, the second smallest positive eigenvalue of (DP) becomes the smallest positive eigenvalue of the new problem. Since the new transformed quadratic eigenproblem has the symmetric positive semidefinite matrix A (see below), in order to distinguish it from (DP) we call this new problem (SP). Since some of the eigenvalue curves as in (1.3) and (1.4) for the problem (SP) can be infinity, in the next section we will show the strictly decreasing property and the asymptotic behavior of those finite eigenvalue curves. Hence, the iterative methods of Section 2 with some slight modifications can be applied successively to find the 2nd, 3rd, 4th, ... smallest positive eigenvalues of (DP).

Let (μ_0, Y_0) be the simple eigensolution of (DP) as above, with $Y_0^T A_0 Y_0 = I_{m_0}$. Note that we have $F(\mu_0)Y_0 = 0$. Define the matrices A_1 , B_1 , and C_1 as follows:

$$A_1 = A_0 - A_0 Y_0 Y_0^T A_0, \quad (3.1a)$$

$$B_1 = B_0 + \mu_0 (A_0 Y_0 Y_0^T C_0 + C_0 Y_0 Y_0^T A_0), \quad (3.1b)$$

$$C_1 = C_0 - \mu_0^2 C_0 Y_0 Y_0^T C_0. \quad (3.1c)$$

THEOREM 3.1. *Let $\mu_0^2 \neq 1/\theta_j$, where θ_j is the j th smallest eigenvalue of $Y_0^T C_0 Y_0$, $j = 1, \dots, m_0$. Then the quadratic eigenvalue problem*

$$F_1(\lambda)x \equiv (A_1 + \lambda B_1 + \lambda^2 C_1)x = 0 \quad (3.2)$$

has the same eigenvalues as $F_0(\lambda)x \equiv (A_0 + \lambda B_0 + \lambda^2 C_0)x = 0$ except that μ_0 is replaced by zero with multiplicity m_0 and A_1 is positive semidefinite with $\text{rank } A_1 = n - m_0$. Furthermore, if $\mu_0^2 < 1/\theta_{m_0}$, then C_1 is positive definite.

Proof. Since $A_1 Y_0 = 0$ and A_0 is positive definite, by interlacing theorem [12] for symmetric matrices it follows that A_1 is positive semidefinite with $\text{rank } A_1 = n - m_0$. From the identities

$$A_0 Y_0 = -\mu_0 B_0 Y_0 - \mu_0^2 C_0 Y_0, \quad (3.3)$$

we have

$$(A_0 + \lambda B_0 + \lambda^2 C_0)Y_0 = (\lambda - \mu_0)(B_0 + (\lambda + \mu_0)C_0)Y_0. \quad (3.4)$$

From (3.4) and the simple identity $\det(I_n + RS) = \det(I_m + SR)$ (where R and S^T are $n \times m$ matrices) we get

$$\begin{aligned} & \det(A_1 + \lambda B_1 + \lambda^2 C_1) \\ &= \det\{(A_0 + \lambda B_0 + \lambda^2 C_0) \\ & \quad + \mu_0[B_0 + (\lambda + \mu_0)C_0]Y_0 Y_0^T (A_0 - \lambda \mu_0 C_0)\} \\ &= \det\left[F_0(\lambda)\left(I_n + \frac{\mu_0}{\lambda - \mu_0}Y_0 Y_0^T\right)(A_0 - \lambda \mu_0 C_0)\right] \\ &= [\det F_0(\lambda)] \det\left(I_{m_0} + \frac{\mu_0}{\lambda - \mu_0}(I_{m_0} - \lambda \mu_0 Y_0^T C_0 Y_0)\right) \\ &= \frac{\lambda^{m_0}}{(\lambda - \mu_0)^{m_0}} \prod_{j=1}^{m_0} (1 - \mu_0^2 \theta_j) \det F_0(\lambda). \end{aligned} \quad (3.5)$$

Hence, the quadratic eigenvalue problem (3.2) preserves all eigenvalues of (1.1) except that μ_0 is replaced by zero with multiplicity m_0 .

Finally, the matrix $C_1 = C_0 - \mu_0^2 C_0 Y_0 Y_0^T C_0$ is congruent to the matrix $\tilde{C}_1 = I - \mu^2 C_0^{1/2} Y_0 Y_0^T C_0^{1/2}$. Since the eigenvalues of C_1 are $\{1, \dots, 1, 1 - \mu_0^2 \theta_1, \dots, 1 - \mu_0^2 \theta_{m_0}\}$, C_1 is positive definite when $\mu_0^2 < 1/\theta_{m_0}$. ■

In order to show that the (SP) problem $F_1(\lambda)x = 0$ as in (3.2) preserves the eigenvectors of the (DP) problem $F_0(\lambda)x = 0$, we first verify the following lemma.

LEMMA 3.2. *Let (μ_0, Y_0) be the simple eigensolution of $F_0(\lambda)x = 0$ with $Y_0^T A_0 Y_0 = I_{m_0}$ and $\mu_0^2 \neq 1/\theta_j$ as in Theorem 3.1. If (μ_1, Y_1) is another eigensolution of $F_0(\lambda)x = 0$ with $\mu_1 \neq \mu_0$, then*

$$Y_1^T (B_0 + (\mu_0 + \mu_1)C_0)Y_0 = 0 \quad (3.6a)$$

and

$$Y_1^T A_0 Y_0 = \mu_0 \mu_1 Y_1^T C_0 Y_0. \quad (3.6b)$$

Proof. Since

$$A_0 Y_0 + \mu_0 B_0 Y_0 + \mu_0^2 C_0 Y_0 = 0$$

and

$$Y_1^T A_0 + \mu_1 Y_1^T B_0 + \mu_1^2 Y_1^T C_0 = 0,$$

we have

$$Y_1^T A_0 Y_0 + \mu_0 Y_1^T B_0 Y_0 + \mu_0^2 Y_1^T C_0 Y_0 = 0 \quad (3.7a)$$

and

$$Y_1^T A_0 Y_0 + \mu_1 Y_1^T B_0 Y_0 + \mu_1^2 Y_1^T C_0 Y_0 = 0. \quad (3.7b)$$

Then (3.6a) follows by subtracting (3.7a) from (3.7b), and (3.6b) follows by subtracting $\mu_1 \times (3.7a)$ from $\mu_0 \times (3.7b)$. ■

THEOREM 3.3. *Let (μ_0, Y_0) be the simple eigensolution of $F_0(\lambda)x = 0$ with $Y_0^T A_0 Y_0 = I_{m_0}$ and $\mu_0^2 \neq 1/\theta_j$ as in Theorem 3.1. Then $F_1(0)Y_0 = 0$, i.e., $(0, Y_0)$ is a simple eigensolution of (3.2) with multiplicity m_0 . If (μ_1, Y_1) is a simple eigensolution of $F_0(\lambda)x = 0$ with $\mu_1 \neq \mu_0$, and $Y_1 \in \mathbb{R}^{n \times m_1}$ with $\text{rank } Y_1 = m_1$, where m_1 is the multiplicity of μ_1 , then (μ_1, Y_1) is a simple eigensolution of $F_1(\lambda)x = 0$ with μ_1 having the same multiplicity m_1 . Therefore, if $F_0(\lambda)$ is a simple λ -matrix, then $F_1(\lambda)$ is also a simple λ -matrix.*

Proof. From (3.1a) and the normalization $Y_0^T A_0 Y_0 = I_{m_0}$, $F_1(0)Y_0 = 0$ follows immediately. From Theorem 3.1 we have that $F_1(\lambda)$ has the same eigenvalues with the same multiplicities as $F_0(\lambda)$ except μ_0 is replaced by 0.

Suppose that $F_0(\mu_1)Y_1 = 0$ with $\text{rank } Y_1 = m_1$, where m_1 is the multiplicity of μ_1 and $\mu_1 \neq \mu_0$. Then

$$\begin{aligned}
 F_1(\mu_1)Y_1 &= (A_1 + \mu_1 B_1 + \mu_1^2 C_1)Y_1 \\
 &= (A_0 + \mu_1 B_0 + \mu_1^2 C_0)Y_1 - A_0 Y_0 (Y_0^T A_0 Y_1) \\
 &\quad + \mu_0 \mu_1 [C_0 Y_0 (Y_0^T A_0 Y_1) + A_0 Y_0 (Y_0^T C_0 Y_1)] \\
 &\quad - \mu_0^2 \mu_1^2 C_0 Y_0 (Y_0^T C_0 Y_1) \\
 &= F_0(\mu_1)Y_1 - (Y_0^T A_0 Y_1 - \mu_0 \mu_1 Y_0^T C_0 Y_1) A Y_0 \\
 &\quad + \mu_0 \mu_1 (Y_0^T A_0 Y_1 - \mu_0 \mu_1 Y_0^T C_0 Y_1) C_0 Y_0 \\
 &= 0
 \end{aligned} \tag{3.8}$$

by Lemma 3.2. The proof is completed. ■

REMARK.

(a) From Theorems 3.1 and 3.3, we see that the nonequivalence deflation (3.1) allows us to transform the original problem (DP) to a new problem (SP) which has the same eigenvalues and their associated eigenvectors as (DP) except that μ_0 is replaced by zero. Note that the deflation (3.1) is not equal to a generalized Wielandt deflation. In fact, we may transform the original problem (DP) to an enlarged linear eigenvalue problem as in (1.2) and derive a generalized Wielandt deflation by applying the same deflation technique as in [13]. Because of the disadvantage in using the problem (1.2) to solve (DP)

that was mentioned in Section 1, we have to transform this generalized Wielandt deflation (of an new enlarged linear eigenvalue problem) back to a quadratic eigenvalue problem. Hence, we can get a so-called quadratic Wielandt deflation for the problem (DP). But we shall see that this quadratic Wielandt deflation is more complex than the deflation (3.1). The quadratic Wielandt deflation is needed to solve several liner systems before deflating the computed eigenvalue of (DP). Besides, the symmetry and positivity of the new transformed matrices are destroyed. Therefore, we prefer using the deflation (3.1) rather than the quadratic Wielandt deflation.

(b) On the other hand, from (3.5) there is also an equivalent form of the deflation (3.1) as follows:

$$F_1(\lambda) = F_0(\lambda) \left(I_n + \frac{\mu_0}{\lambda - \mu_0} Y_0 Y_0^T (A_0 - \lambda \mu_0 C_0) \right). \quad (3.9)$$

The roundoff errors on performing (3.9) will become large when λ is close to μ_0 . Moreover, the symmetry and the positivity properties for $F_1(\lambda)$ can be lost if we perform (3.9) directly. Therefore, we still prefer using (3.1) rather than (3.9).

In the following, we extend Theorem 3.1 and 3.3.

THEOREM 3.4. *Let $(\mu_0, Y_0), \dots, (\mu_r, Y_r)$ be the simple eigensolutions of $F_0(\lambda)x = 0$ with μ_j having multiplicity m_j , $j = 0, \dots, r$. Suppose that $Y^T A_0 Y = I_{\sigma_r}$, where $Y \equiv [Y_0, \dots, Y_r]$ and $\sigma_r = m_0 + \dots + m_r$, and $\mu_j^2 < 1/\theta_{m_j}$ with $\theta_{m_j} = \lambda_{\max}(Y_j^T C_0 Y_j)$, $j = 0, \dots, r$. Then for $j = 0, 1, \dots, r$*

$$A_{j+1} = A_j - A_j Y_j Y_j^T A_j, \quad (3.10a)$$

$$B_{j+1} = B_j + \mu_j (A_j Y_j Y_j^T C_j + C_j Y_j Y_j^T A_j), \quad (3.10b)$$

$$C_{j+1} = C_j - \mu_j^2 C_j Y_j Y_j^T C_j \quad (3.10c)$$

are well defined. Further, A_{j+1} is positive semidefinite with nullity $\sigma_j \equiv m_0 + \dots + m_j$ satisfying

$$Y^T A_{j+1} Y = 0_{m_0} \oplus \dots \oplus 0_{m_j} \oplus I_{m_{j+1}} \oplus \dots \oplus I_{m_r},$$

and C_{j+1} is positive definite. Let

$$F_j(\lambda) \equiv A_j + \lambda B_j + \lambda^2 C_j, \quad j = 0, 1, \dots, r.$$

Then for $j = 0, 1, \dots, r$

$$F_{j+1}(0)Y_l = 0, \quad l = 0, 1, \dots, j,$$

and

$$F_{j+1}(\mu_l)Y_l = 0, \quad l = j + 1, \dots, r.$$

Proof. The theorem is obtained by induction. The proof is similar to that of Theorem 3.3; we omit the details. \blacksquare

4. ANALYSIS OF EIGENVALUE CURVES $\beta(\lambda)$ FOR THE (SP) PROBLEM

For the generalization of the three iterative methods in Section 2 to find the smallest positive eigenvalue of an (SP) problem derived by the nonequivalence deflation (3.1), we shall analyze the asymptotic behavior and show the decreasing property of eigenvalue curves $\beta(\lambda)$ represented by

$$\beta(\lambda)Ax(\lambda) = -(B + \lambda C)x(\lambda), \quad (4.1)$$

where A is positive semidefinite. The eigenvalue curves $\beta(\lambda)$ here are allowed to be $\pm\infty$. Suppose that

$$\dim \mathcal{N}(A) = k > 0 \quad (4.2a)$$

and

$$\mathcal{N}(A) \cap \mathcal{N}(B + \lambda C) = \{0\} \quad \text{for all } \lambda \in \mathbb{R}. \quad (4.2b)$$

Here $\mathcal{N}(A)$ denotes the null space of A . Let X_k be an orthogonal basis of $\mathcal{N}(A)$, i.e., $AX_k = 0$ and $X_k^T X_k = I_k$. Since the matrix C is positive definite, the polynomial

$$f_k(\lambda) \equiv -\det(X_k^T B X_k + \lambda X_k^T C X_k) \quad (4.3)$$

has k real roots as follows:

$$\underbrace{\gamma_1 = \dots = \gamma_1}_{\nu_1} < \underbrace{\gamma_2 = \dots = \gamma_2}_{\nu_2} < \dots < \underbrace{\gamma_l = \dots = \gamma_l}_{\nu_l}, \quad (4.4)$$

with $\nu_1 + \dots + \nu_l = k$. Let $r = n - k$, and $s_j = \nu_{j+1} + \dots + \nu_l$, for $j = 0, \dots, l - 1$. For a fixed $\lambda \in (\gamma_j, \gamma_{j+1})$, $j = 0, \dots, l$, the matrix $-(X_k^T B X_k +$

$\lambda X_k^T C X_k) \equiv M_k(\lambda)$ is nonsingular. (Here, for convenience we set $\gamma_0 = -\infty$ and $\gamma_{l+1} = \infty$, respectively.) Furthermore, it is easily seen that

$$M_k(\lambda) \text{ is congruent to } I_{s_i} \oplus (-I_{k-s_j}). \quad (4.5)$$

From Theorem 4.1 of [9] and the assumption (4.2) it follows that there is a nonsingular matrix $X(\lambda)$ such that

$$X^T(\lambda) A X(\lambda) = I_r \oplus O_k \quad (r = n - k) \quad (4.6a)$$

and

$$\begin{aligned} & -X^T(\lambda)(B + \lambda C)X(\lambda) \\ & = \text{diag}\{\beta_{s_j+1}(\lambda), \dots, \beta_{s_j+r}(\lambda)\} \oplus I_{s_j} \oplus (-I_{k-s_j}). \end{aligned} \quad (4.6b)$$

Hence, for a given $\lambda \in (\gamma_j, \gamma_{j+1})$, the symmetric linear eigenvalue problem (4.1) has finite and infinite eigenvalues labeled as follows:

$$\underbrace{\infty = \dots = \infty}_{s_j} > \beta_{s_j+1}(\lambda) \geq \dots \geq \beta_{s_j+r}(\lambda) > \underbrace{-\infty = \dots = -\infty}_{k-s_j}. \quad (4.7)$$

We now consider the case $\lambda = \gamma_j$, for $j = 1, \dots, l$. From (4.3) and (4.4) it is easily seen that

$$M_k(\gamma_j) \text{ is congruent to } I_{s_j} \oplus O_{\nu_j} \oplus (-I_{k-s_{j-1}}). \quad (4.8)$$

By Theorem 4.1 of [9] and the assumption (4.2) again, there is a nonsingular matrix $X(\gamma_j)$ such that

$$X^T(\gamma_j) A X(\gamma_j) = I_{r-\nu_j} \oplus \underbrace{\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \oplus \dots \oplus \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}}_{\nu_j} \oplus O_{k-\nu_j} \quad (4.9a)$$

and

$$\begin{aligned} & -X^T(\gamma_j)(B + \gamma_j C)X(\gamma_j) \\ & = \text{diag}\{\beta_{s_{j-1}+1}(\gamma_j), \dots, \beta_{s_j+r}(\gamma_j)\} \\ & \quad \oplus \underbrace{\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \oplus \dots \oplus \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}}_{\nu_j} \oplus I_{s_j} \oplus (-I_{k-s_{j-1}}). \end{aligned} \quad (4.9b)$$

Hence, for $\lambda = \gamma_j$, the finite and infinite eigenvalues of the problem (4.1) can be labeled as follows:

$$\underbrace{\infty = \cdots = \infty}_{s_{j-1}} > \beta_{s_{j-1}+1}(\gamma_j) \geq \cdots \geq \beta_{s_j+r}(\gamma_j) > \underbrace{-\infty = \cdots = -\infty}_{k-s_{j-1}}. \quad (4.10)$$

Note that, from (4.9), we see that there are ν_j 2×2 Jordan blocks corresponding to the matrix pair $(-B - \gamma_j C, A)$. Hence, there are only $r - \nu_j$ eigenvalues in (4.10).

We now study the local behavior of eigenvalue curves $\beta(\lambda)$ in (4.1). We consider the characteristic equation

$$\det[\beta(\lambda)A + B + \lambda C] = 0. \quad (4.11)$$

Since A is positive semidefinite with $\text{rank } A = r \equiv n - k$, (4.11) can be written as

$$a_k(\lambda)\beta(\lambda)^r + a_{k+1}(\lambda)\beta(\lambda)^{r-1} + \cdots + a_{n-1}(\lambda)\beta(\lambda) + a_n(\lambda) = 0, \quad (4.12)$$

where $a_k(\lambda) = \alpha f_k(\lambda)$ with $\alpha \equiv \text{constant} \neq 0$. For any $\lambda \in (\gamma_j, \gamma_{j+1})$, $j = 0, 1, \dots, l$, the equation (4.12) has r roots $\beta_{s_{j+1}}(\lambda), \dots, \beta_{s_j+r}(\lambda)$ corresponding to those eigenvalues in (4.7). By a well-known result on algebraic functions (see for example [27, p. 65]) the derivatives of the roots $\beta_i(\lambda)$ of (4.12) exist and are continuous at each $\lambda \in (\gamma_j, \gamma_{j+1})$ except possibly a finite number of points where the derivatives of $\beta_i(\lambda)$ may be discontinuous. For the point $\lambda = \gamma_j$, $j = 1, \dots, l$, the canonical decompositions (4.9) show that the matrix pair $(-B - \gamma_j C, A)$ has only $r - \nu_j$ finite eigenvalues. Hence the equation (4.12) becomes

$$a_{k+\nu_j}(\gamma_j)\beta(\gamma_j)^{r-\nu_j} + \cdots + a_{n-1}(\gamma_j)\beta(\gamma_j) + a_n(\gamma_j) = 0 \quad (4.13)$$

with $a_k(\gamma_j) = \cdots = a_{k+\nu_j-1}(\gamma_j) = 0$ and $a_{k+\nu_j}(\gamma_j) \neq 0$. The equation (4.13) has $r - \nu_j$ roots $\beta_{s_{j-1}+1}(\gamma_j), \dots, \beta_{s_j+r}(\gamma_j)$ corresponding to those eigenvalues in (4.10). By the same argument as above we see that $\beta'_i(\lambda)$ exists for $i = s_{j-1} + 1, \dots, s_j + r$, except possibly at a finite number of points. From the above discussion we see that the derivatives of the eigenvalue curves $\beta(\lambda)$ in (4.1) exist almost everywhere. The following theorem, similar to an earlier result of [15], gives a representation formula of $\beta'(\lambda)$. Note that $x(\lambda)$ in (4.1) is differentiable at λ if $\beta'(\lambda)$ exists.

THEOREM 4.1. *If $\beta'(\lambda)$ exists and there is an $x(\lambda)$ with $x^T(\lambda)Ax(\lambda) = 1$ such that (4.1) holds, then*

$$\beta'(\lambda) = -x^T(\lambda)Cx(\lambda). \quad (4.14)$$

Therefore, the function $\beta(\lambda)$ is strictly decreasing and satisfies $-\lambda_{\max}(C) \leq \beta'(\lambda) \leq -\lambda_{\min}(C)$.

Proof. Let $\lambda \in (\gamma_j, \gamma_{j+1})$ for some $j \in \{0, 1, \dots, l\}$. According to (4.6), the columns $\{x_i^{(j)}(\lambda)\}$ of $X(\lambda)$ form a linearly independent basis and satisfy

$$\beta_{s_j+i}(\lambda) Ax_i^{(j)}(\lambda) = -(B + \lambda C)x_i^{(j)}(\lambda) \quad (4.15a)$$

with

$$x_i^{(j)}(\lambda)^T Ax_i^{(j)}(\lambda) = 1 \quad (4.15b)$$

for $i = 1, \dots, r$. Hence, the eigenpair $(\beta(\lambda), x(\lambda))$ as in (4.1) must be equal to an eigenpair $(\beta_{s_j+i_0}(\lambda), x_{i_0}^{(j)}(\lambda))$ for some $i_0 \in \{1, \dots, r\}$. Taking the inner product of (4.15a) with $x(\lambda)$ and making use of the normalization (4.15b), we obtain

$$\beta(\lambda) = -x(\lambda)^T Bx(\lambda) - \lambda x(\lambda)^T Cx(\lambda). \quad (4.16)$$

Differentiating (4.16) with respect to λ gives

$$\beta'(\lambda) = -2x(\lambda)^T (B + \lambda C)x'(\lambda) - x(\lambda)^T Cx(\lambda). \quad (4.17)$$

Since $x(\lambda)^T Ax'(\lambda) = 0$, from (4.6a) we see that $x'(\lambda)$ can be expressed as

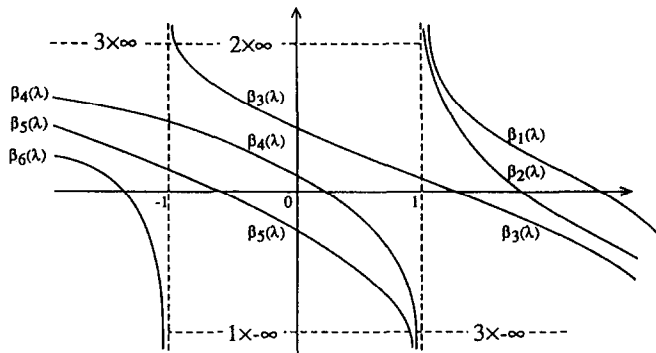
$$x'(\lambda) = \sum_{\substack{i=1 \\ i \neq i_0}}^n c_i x_i^{(j)}(\lambda), \quad (4.18)$$

for some constant scalars c_1, \dots, c_n . Substituting (4.18) into (4.17) and using (4.6b), we obtain that (4.14) holds for $\lambda \in (\gamma_j, \gamma_{j+1})$, $j = 0, 1, \dots, l$.

For the case $\lambda = \gamma_j$ with $j \in \{1, \dots, l\}$, from (4.9a, b), if we let

$$X(\gamma_j) = [x_1^{(j)}(\gamma_j), \dots, x_n^{(j)}(\gamma_j)],$$

then the eigenpair $(\beta(\lambda), x(\lambda))$ is equal to the pair $(\beta_{s_{j-1}+i_0}(\gamma_j), x_{i_0}^{(j)}(\gamma_j))$ for some $i_0 \in \{1, \dots, r - \nu_{j_0}\}$. By using the same arguments as in (4.16)–(4.18), we get the assertion (4.14) at $\lambda = \gamma_j$, $j = 1, \dots, l$. ■

FIG. 1. The functions $\beta(\lambda)$.

The graph of eigenvalue curves $\beta(\lambda)$ is probably best illustrated by an example. Suppose the matrix A , of order 6, has rank 3, and let $\gamma_1 = -1$ with $\nu_1 = 1$ and $\gamma_2 = 1$ with $\nu_2 = 2$. According to the strictly decreasing property of $\beta(\lambda)$ from Theorem 4.1, the graph of $\beta(\lambda)$ for this example is as shown in Figure 1.

We now exploit the decreasing property of $\beta(\lambda)$ and the representation formula (4.14) of $\beta'(\lambda)$ to generalize three iterative methods in Section 2 for finding the smallest positive eigenvalue of the (SP) problem.

Suppose that the smallest positive eigenvalue, say λ_* , of the (SP) problem satisfies

$$\gamma_m < 0 < \lambda_* < \gamma_{m+1} \quad (4.19)$$

for some $m \in \{0, \dots, l\}$. Then the eigenvalue λ_* is the fixed point of the function $1/\beta_{s_{m+1}}(\lambda)$. Note that for the problem (DP) the condition (4.19) is automatically satisfied ($k = l = 0$) and the eigenvalue λ_* is the fixed point of the function $1/\beta_1(\lambda)$.

Given an (SP) problem satisfying the conditions (4.2). The following three iterative methods find the smallest positive eigenvalue λ_* which satisfies (4.19).

BASIC ITERATIVE METHOD (SP).

0. If $\gamma_j = 0$ for some $j \in \{1, \dots, l\}$, then fail and stop, else let $m \in \{0, \dots, l\}$ such that $\gamma_m < 0 < \gamma_{m+1}$.
1. Given a suitable initial guess $\lambda_0 \geq 0$. Let $p = 0$.

Repeat:

2. Call Subroutine NTL to compute the eigenpair $(\beta_{s_m+1}(\lambda_p), x_1(\lambda_p))$ of the generalized eigenvalue problem

$$\beta(\lambda_p)Ax(\lambda_p) = -(B + \lambda_p C)x(\lambda_p).$$

3. Let $\lambda_{p+1} = 1/\beta_{s_m+1}(\lambda_p)$.
4. If $\lambda_{p+1} \geq \gamma_{m+1}$, then fail and stop.
5. If $|\lambda_{p+1} - \lambda_p| \leq \text{Tolerance}$, then
 set $\lambda_* = \lambda_{p+1}$ and stop,
 else $p := p + 1$, $\lambda_p := \lambda_{p+1}$, goto Repeat.

SUBROUTINE NTL (Noncongruence transformation + Lanczos method).
 Let $M := -(B + \lambda_p C)$ and $AX_k = 0$ with $X_k^T X_k = I_k$. This subroutine computes the largest positive eigenvalue β excluding ∞ of the eigenvalue problem $\beta Ax = Mx$.

1. Compute the spectrum decomposition of $H \equiv X_k^T M X_k$ by applying QR iteration:
 $W^T H W = \text{diag}\{\sigma_1, \dots, \sigma_k\}$ [$\sigma_i \neq 0$ for all i by the condition (4.19)].
2. Let $Z_k := X_k \text{diag}\{|\sigma_1|^{-1/2}, \dots, |\sigma_k|^{-1/2}\} \equiv [z_1, \dots, z_k]$.
 Compute $S := \text{diag}\{\text{sgn}(z_1^T M z_1), \dots, \text{sgn}(z_k^T M z_k)\}$.
3. Form $\hat{A} := A + M Z_k Z_k^T M$ [which is nonsingular by (4.6)] and $\hat{M} := M - M Z_k S Z_k^T M$.
4. Perform the symmetric Lanczos algorithm [19, p. 323] on the matrix $\hat{A}^{-1} \hat{M}$ to compute the largest positive eigenvalue β_{l_p} and the associated eigenvector x_{l_p} .
 Set $\beta_{s_m+1}(\lambda_p) := \beta_{l_p}$ and $x_1(\lambda_p) := x_{l_p}$, return.

Note that from [13] the eigenvectors of the pair (\hat{A}, \hat{M}) are the same as (A, M) .

To implement the Lanczos algorithm at step 4 above, it is necessary to solve a linear system $\hat{A}y = c$. If the matrix A is written as

$$A = A_0 - Y_k Y_k^T, \quad Y_k \in \mathbb{R}^{n \times k},$$

where A_0 is symmetric positive definite and the LDL^T factorization of A_0 is known, then the transformed matrix \hat{A} in step 3 is a low-rank updating of A_0 . That is, $\hat{A} = A_0 + UV^T$, where $U = [-Y_k, MZ_k]$ and $V = [Y_k, MZ_k]$. Since \hat{A} is symmetric positive definite,

(a) the Sherman-Morrison-Woodbury formula

$$(A_0 + UV^T)^{-1} = A_0^{-1} - A_0^{-1}U(I + V^T A_0^{-1}U)^{-1}V^T A_0^{-1}$$

exists and can be used to solve the linear system $\hat{A}y = c$;

(b) an MDR technique [5] can be applied to compute a factorization of \hat{A} by using the LDL^T factorization of A_0 and the low-rank updating formula $\hat{A} = A_0 + UV^T$.

TANGENT ITERATIVE METHOD (SP).

0. If $\gamma_j = 0$ for some $j \in \{1, \dots, l\}$, then fail and stop,
else let $m \in \{0, \dots, l\}$ such that $\gamma_m < 0 < \gamma_{m+1}$.
1. Given a suitable initial guess $\lambda_0 \geq 0$. Let $p = 0$.
Repeat:
2. Call Subroutine NTL to compute the eigenpair $(\beta_{s_{m+1}}(\lambda_p), x_1(\lambda_p))$ of the eigenproblem

$$\beta(\lambda_p) Ax(\lambda_p) = -(B + \lambda_p C)x(\lambda_p),$$

Let $\beta_*(\lambda_p) \equiv \beta_{s_{m+1}}(\lambda_p)$.

3. Compute $b(\lambda_p) = \beta_*(\lambda_p) - \beta'_*(\lambda_p)\lambda_p$ and $c(\lambda_p) = b(\lambda_p)^2 + 4\beta'_*(\lambda_p)$, where
 $\beta'_*(\lambda_p) := -x_1(\lambda_p)^T C x_1(\lambda_p)$.
4. If $c(\lambda_p) \geq 0$, then
compute $\lambda_{p+1} = \{-b(\lambda_p) + [\text{sgn } b(\lambda_p)]\sqrt{c(\lambda_p)}\}/2\beta'_*(\lambda_p)$,
else $\lambda_{p+1} = 1/\beta_*(\lambda_p)$ (basic iteration).
5. If $\lambda_{p+1} \geq \gamma_{m+1}$, then fail and stop.
6. If $|\lambda_{p+1} - \lambda_p| \leq \text{Tolerance}$, then
set $\lambda_* := \lambda_{p+1}$ and stop,
else $p := p + 1$, $\lambda_p := \lambda_{p+1}$, goto Repeat.

Newton Iterative Method (SP).

0. If $\gamma_j = 0$ for some $j \in \{1, \dots, l\}$, then fail and stop,
else let $m \in \{0, \dots, l\}$ such that $\gamma_m < 0 < \gamma_{m+1}$.
1. Given a suitable initial guess $\lambda_0 \geq 0$. Let $p = 0$.
Repeat:
2. Call subroutine NTL to compute the eigenpair $(\beta_{s_{m+1}}(\lambda_p), x_1(\lambda_p))$ of the eigenproblem

$$\beta(\lambda_p) Ax(\lambda_p) = -(B + \lambda_p C)x(\lambda_p).$$

Let $\beta_*(\lambda_p) \equiv \beta_{s_{m+1}}(\lambda_p)$.

3. Let $r_p = -\beta'_*(\lambda_p)/\beta^2_*(\lambda_p) = x_1(\lambda_p)^T C x_1(\lambda_p)/\beta^2_*(\lambda_p)$.
4. If $r_p < 1$, then
Compute $\lambda_{p+1} = [\lambda_p \beta'_*(\lambda_p) + \beta_*(\lambda_p)]/[\beta^2_*(\lambda_p) + \beta'_*(\lambda_p)]$.
else if $r_p = 1$ and $\lambda_p = 1/\beta_*(\lambda_p)$, then stop,
else $\lambda_{p+1} = 1/\beta_*(\lambda_p)$ (basic iteration).

5. If $\lambda_{p+1} \geq \gamma_{m+1}$, then fail and stop.
6. If $|\lambda_{p+1} - \lambda_p| \leq \text{Tolerance}$, then
 set $\lambda_* := \lambda_{p+1}$ and stop,
 else $p := p + 1$, $\lambda_p := \lambda_{p+1}$, goto Repeat.

We can also prove the linear convergence rate of the basic iterative method (SP), and the quadratical convergence rate of the tangent and Newton iterative methods (SP), as in Section 2.

For the initial guess, we have some comments as follows. Since the Theorem 4.1 the eigenvalue curves $\beta(\lambda)$ are strictly decreasing and differentiable almost everywhere, we see that $1/\beta_{s_m+1}(0)$ is a good initial guess in iterative methods for finding the smallest positive fixed point of $1/\beta_{s_m+1}(\lambda)$. On the other hand, if the condition (4.19) is not satisfied, i.e., if there is a $\gamma_{m+1} \in (0, \lambda_*)$, then $1/\beta_{s_m+1}(0)$ is not suitable as an initial value. Because in this case λ_* is the fixed point of the function $1/\beta_{s_m+1}(\lambda)$ and $\beta_{s_m+1}(\lambda_*) > \beta_{s_m+1}(\lambda_*)$, we get the wrong fixed point if we follow the curve $\beta_{s_m+1}(\lambda)$ by using the initial value $1/\beta_{s_m+1}(0)$.

If we follow the eigenvalue curve $\beta(\lambda)$ by using iterative methods developed above for finding the largest positive eigenvalue $\beta(\lambda_p)$ at the current λ_p ($p = 0, 1, \dots$), then we can possibly follow the curve $\beta_{s_m+1}(\lambda)$ at $\lambda = \lambda_p > \gamma_{m+1}$ and $\beta_{s_m+1}(\lambda)$ at $\lambda = \lambda_p < \gamma_{m+1}$, respectively. But $\beta_{s_m+1}(\gamma_{m+1} + \varepsilon) \rightarrow \infty$ and $\beta_{s_m+1}(\gamma_{m+1} - \varepsilon) < \infty$ (bounded) as $\varepsilon \rightarrow 0^+$, since the Kronecker structure at the point near γ_{m+1} of the form (4.6) or (4.9) is very sensitive [26]. The graph of this case is shown in Figure 2. Therefore, our iterative methods fail for this case. Fortunately, in our numerical experiments the desired positive eigenvalues have been found before we meet this case.

5. NUMERICAL ALGORITHM AND EXAMPLES

In this section, we develop an algorithm for finding a few of the smallest positive eigenvalues of (DP) by using the iterative methods proposed in Section 4 combined with the nonequivalence deflation technique (in Section 3). Here, we assume that the desired positive eigenvalues are simple, namely, the multiplicity of each desired eigenvalue is equal to the dimension of the subspace spanned by its associated eigenvectors.

ALGORITHM 5.1 (Basic tangent-Newton iteration + nonequivalence deflation). Given $F_0(\lambda) \equiv A_0 + \lambda B_0 + \lambda^2 C_0$ with A_0, C_0 symmetric positive definite and B_0 symmetric. Given a positive integer $d \ll n$. Find the smallest d positive eigenvalues of $F_0(\lambda)$ and their associated eigenvectors.

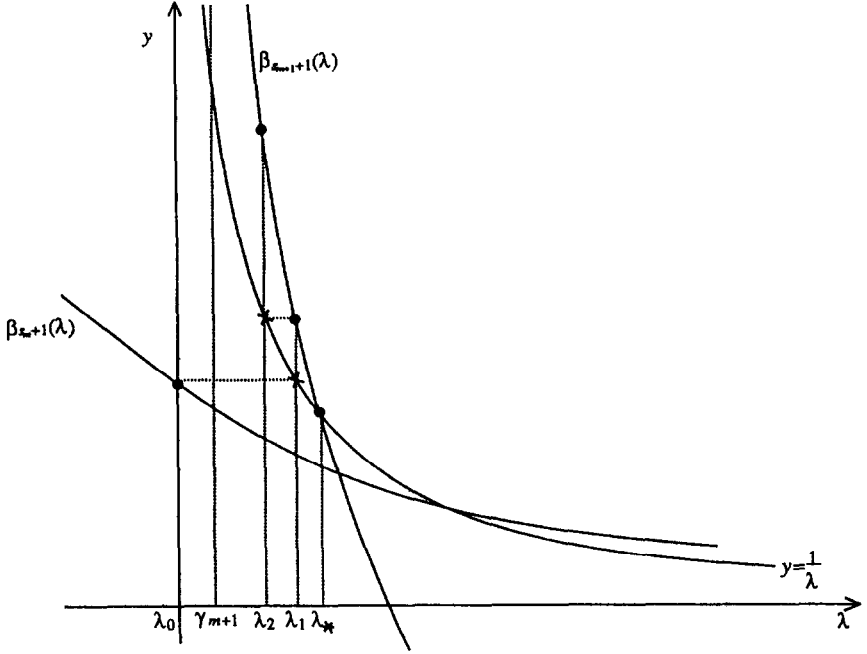


FIG. 2.

0. Compute the Cholesky decomposition of A_0 , $A_0 = L_0 D_0 L_0^T$. Let $\lambda_0 = 0$ and $\gamma_* = \infty$.

For $i = 0, 1, \dots, d - 1$, do:

$j = 0$.

1. Repeat:

1.1. Call Subroutine NTL (in Section 4) to compute the largest finite eigenpair (β, Ψ) of $(B_i + \lambda_j C_i)$

1.2. Update λ_{j+1} by tangent-Newton step or basic step.

If $\lambda_{j+1} \geq \gamma_*$, then fail and stop.

If $|\lambda_{j+1} - \lambda_j| \leq \text{Tolerance}$, then

set $\mu_i = \lambda_{j+1}$,

$Y_i = \Psi \in \mathbb{R}^{n \times m_i}$, where m_i is the multiplicity of β .

$X_i \equiv [Y_0, \dots, Y_i]$.

go to 2.

else

$\lambda_j = \lambda_{j+1}$, $j = j + 1$, go to Repeat.

2. Three criteria:

2.1. Compute $\gamma_* :=$ the smallest nonnegative eigenvalue of matrix pair $(X_i^T B_i X_i, -X_i^T C_i X_i)$.

If

$$\mu_i \geq \gamma_*, \quad (5.1)$$

then fail and stop.

2.2. Compute the spectrum decomposition of $H_i \equiv Y_i^T A_i Y_i$ such that

$$S_i^T H_i S_i = \text{diag}\{\delta_1^{(i)}, \dots, \delta_{m_i}^{(i)}\} = D_i,$$

where $S_i = [s_1^{(i)}, \dots, s_{m_i}^{(i)}]$ is an $m_i \times m_i$ orthogonal matrix.

If there exists an $l \in \{1, \dots, m_i\}$ such that

$$\delta_l^{(i)} = 0, \quad (5.2)$$

then fail and stop.

2.3. Let $\tilde{Y}_i = Y_i S_i D_i^{-1/2}$. Compute the spectrum of $\tilde{Y}_i^T C_i \tilde{Y}_i = \{\theta_1^{(i)}, \dots, \theta_{m_i}^{(i)}\}$ with $\theta_1^{(i)} \leq \dots \leq \theta_{m_i}^{(i)}$.

If

$$\mu^2 \geq \frac{1}{\theta_{m_i}}, \quad (5.3)$$

then fail and stop.

3. Nonequivalence deflation:

Compute $\tilde{U}_i := A_i \tilde{Y}_i$ and $\tilde{V}_i := \mu_i C_i \tilde{Y}_i$.

Define $U_i = [\tilde{U}_0, \dots, \tilde{U}_i]$ and $V_i = [\tilde{V}_0, \dots, \tilde{V}_i]$.

Form

$$A_{i+1} := A_0 - U_i U_i^T,$$

$$B_{i+1} := B_0 + U_i V_i^T + V_i U_i^T,$$

$$C_{i+1} := C_0 - V_i V_i^T.$$

Endfor

COMMENT ON STEP 2. The criterion (5.1) is according to (4.19). Since A_i is symmetric positive semidefinite with $\mathcal{M}(A_i) = \text{span}\{Y_0, \dots, Y_{i-1}\}$, $H_i = Y_i^T A_i Y_i$ is also symmetric positive semidefinite. If there is a $\delta_l^{(i)} = 0$ for some $l \in \{1, \dots, m_i\}$, then $Y_i s_l^{(i)} \in \mathcal{M}(A_i)$. Hence, according to Theorem 3.4, the criterion (5.2) is to check the linear independence of the desired eigenvectors

$\{Y_0, \dots, Y_{d-1}\}$. The criterion (5.3) guarantees the next transformed matrix C_{i+1} is positive definite according to Theorem 3.4.

COMMENT ON STEP 3. The nonequivalence-deflation updating formulae in step 3 are identical to the formulae in (3.10). Since the Cholesky decomposition of A_0 is known, the representation of the inverse of A_{i+1} is convenient for the Sherman-Morrison-Woodbury formula or MDR technique mentioned in the comment of Subroutine NTL in Section 4.

We tested Algorithm 5.1 on several examples by using MATLAB (16 digits) on a Sparc Station 10 computer.

In Section 1 we mentioned that the unsymmetric Lanczos method [7, 21] can be applied to the matrix

$$\begin{bmatrix} B & A \\ A & O \end{bmatrix}^{-1} \begin{bmatrix} -C & O \\ O & A \end{bmatrix}$$

for finding the extreme eigenvalues $\mu \equiv 1/\lambda$ of (1.2). If the reciprocals of the desired positive eigenvalues are surrounded by a lot of reciprocals of the complex conjugate eigenvalues, then the Lanczos method may not converge to the desired reciprocals μ . On the contrary, Algorithm 5.1 can directly find out the desired positive eigenvalues.

EXAMPLE 5.1. In this example we simulate a shall buckling model with large deflection by using the finite-element method [2, 6]. The corresponding quadratic eigenvalue problem is described as

$$\left[K_0 + \lambda_{\text{cr}} N1(u)|_{u=u_{\text{ref}}} + \lambda_{\text{cr}}^2 N2(u^2)|_{u=u_{\text{ref}}} \right] u = 0, \quad (5.4)$$

where λ_{cr} is the critical load, u_{ref} is a reference displacement vector, and u is the generalized displacement (buckled mode shape). Furthermore, the matrix K_0 is the linear stiffness matrix

$$\int_V B_0^T E B_0 dV > 0;$$

the matrix $N1(u)$ is the stiffness matrix linearly dependent on the generalized displacement,

$$\int_V B_0^T E B_L(u) dV + \int_V B_L(u)^T E B_0 dV + \int_V \frac{dB_L^T(u)}{du} \sigma dV;$$

and the matrix $N2(u^2)$ is the stiffness matrix quadratically dependent on u ,

$$\int_V B_L^T(u) E B_L(u) dV > 0.$$

Here, E is the elasticity matrix, σ is the stress, and ε is the strain, which satisfy the elastic relation

$$\sigma = E(\varepsilon - \varepsilon_0) + \sigma_0.$$

Besides, the strain ε depends nonlinearly on the displacement according to the strain condition

$$d\varepsilon = B(u) du,$$

where $B(u) \equiv B_0 + B_L(u)$ is dependent on u .

Since the off-diagonal entries of three matrices in (5.4) are much smaller in modulus than the corresponding diagonal entries, for simplification of computations we consider the quadratic eigenvalue problem (1.1) with $A = \text{diag}(K_0)$, $B = \text{diag}[N1(u)|_{u=u_{\text{ref}}}]$, and $C = \text{diag}[N2(u^2)|_{u=u_{\text{ref}}}]$. The dimension n of A , B , and C is 1407. The distribution of the reciprocals of the eigenvalues of (1.1) is shown in Figure 3. It can be shown that the reciprocals of the eigenvalues have in modulus the following order:

$$70c > 8r > 20c > 1r > 40c > 1r > 20c > 6r.$$

This means that 70 reciprocals of complex eigenvalues are larger in modulus than 8 reciprocals of positive real eigenvalues, 8 reciprocals of positive real eigenvalues are larger in modulus than 20 reciprocals of complex eigenvalues, and so on.

We now apply Algorithm 5.1 to this example. Table 1 shows that the smallest positive eigenvalues can successively be found until the criterion (5.1) holds. The second column of Table 1 records the number of tangent-Newton iterations (combined with basic iteration), the third column records the number of corresponding block Lanczos steps with block size in parentheses, the fourth and fifth column record, respectively, the convergent eigenvalues μ_j and residuals of the convergent eigenpair (μ_j, y_j) , where residual $\equiv \|(A + \mu_j B + \mu_j^2 C)y_j\|_2$, and the last column records the smallest nonnegative eigenvalue γ_* of $(Y_j^T B_j Y_j, -Y_j^T C_j Y_j)$ in the criterion (5.1).

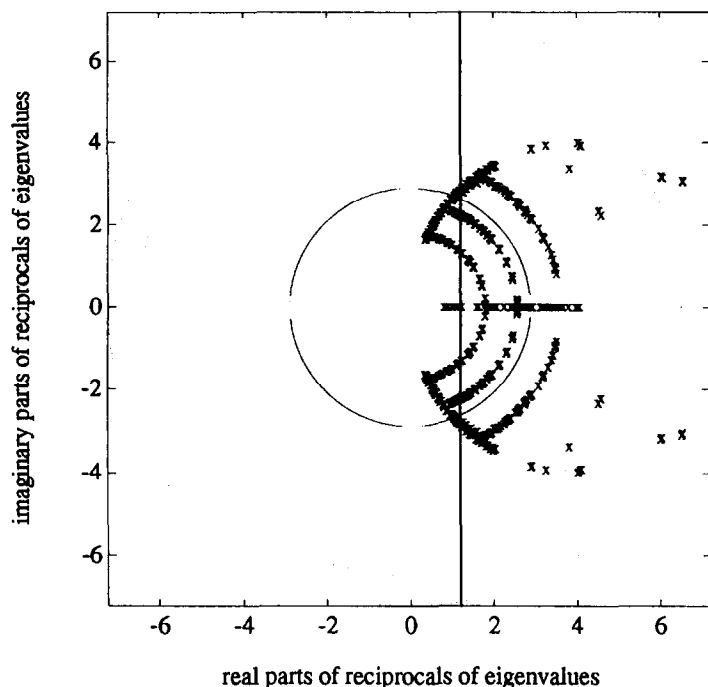


FIG. 3. Reciprocals of the eigenvalues.

Note that the vertical line in Figure 3 denotes the position of $1/\gamma_*$. In Table 1, we see that the tangent-Newton iteration converges very fast. It needs about four steps on average for converging to one positive real eigenvalue. the number of block Lanczos steps is about 28.5 on average for one tangent-Newton iteration. In general, this quantity is independent of the dimension n , but depends on the distribution of the eigenvalues.

In Table 1 many numbers of block Lanczos steps are equal to one. In fact, after performing block Lanczos iterations, we can obtain a subspace spanned by some Ritz vectors. If the iterative value λ_p is very close to a desired eigenvalue λ_* , then this spanned subspace is close to the subspace spanned by the eigenvectors corresponding to some desired eigenvalues. This is like taking the eigenpairs of a perturbed eigenvalue problem as the initial guess of the next block Lanczos iteration. So the Lanczos iteration iteration usually converges to the desired value in one step. In addition, there are other, larger numbers of Lanczos steps among those 1's in Table 1, arising from the intersection of the desired eigencurve with the other eigencurves. Further-

TABLE 1
 $n = 1407$; A , B , AND C ARE DIAGONAL AND GIVEN BY EXAMPLE 5.1

No.	Step	Lanczos no.	Conv. eigenval.	Residual	γ_*
1	9	29,1,1,1,1,40,45,1,1(8)	2.4688E - 01	3.9774E - 11	1.4883
2	4	46,1,1,1(7)	2.4752E - 01	1.6450E - 10	1.2413
3	4	47,1,1,1(6)	2.4851E - 01	5.9319E - 10	1.2382
4	4	48,1,50,1(5)	2.4918E - 01	2.6342E - 15	1.2332
5	4	50,1,1,1(4)	2.4955E - 01	6.2633E - 11	1.2299
6	4	52,1,1,1(3)	2.4962E - 01	1.7139E - 09	1.2281
7	4	49,1,1,1(2)	2.4981E - 01	1.0278E - 09	1.2268
8	4	52,51,53,51(1)	2.4992E - 01	2.1113E - 09	1.2268
9	4	51,1,1,1(8)	2.5224E - 01	2.2948E - 15	1.2263
10	4	55,1,1,1(7)	2.6396E - 01	9.9665E - 13	1.2150
11	4	61,1,1,1(6)	2.7301E - 01	4.7755E - 10	1.1610
12	4	60,63,62,64(5)	2.74118E - 01	6.7313E - 10	1.1226
13	3	69,71,73(4)	2.74125E - 01	2.3301E - 09	1.11804
14	4	81,1,1,1(3)	2.7430E - 01	5.4787E - 10	1.11801
15	4	94,1,1,1(2)	2.7466E - 01	9.9665E - 10	1.1158
16	4	109,107,108,108(1)	2.7480E - 01	1.8419E - 09	1.1158

more, the magnitude of the first value of each row of the number of Lanczos steps yields the spectrum gap ratio. The accuracy of the convergent eigenvalues is at least 10 significant digits.

EXAMPLE 5.2. Given three 100×100 randomly generated symmetric matrices A , B , and C with A, C positive definite and B negative definite. We now consider the quadratic eigenvalue problems

$$(A + \lambda B + \lambda^2 \varepsilon C)x = 0$$

(5.5)

with values $\varepsilon = 5.0, 3.0, 2.0, 0.8$. We plot the distribution of the reciprocals of the eigenvalues of (5.5) with different ε in Figure 4(a)–(d) and show the numerical results to illustrate the functioning of Algorithm 5.1.

In the case $\varepsilon = 5.0$ [Figure 4(a)] the reciprocal of the smallest positive eigenvalue is smaller than the absolute values of 40 reciprocals of complex conjugate eigenvalues. This is the disadvantage of performing the unsymmetric Lanczos method or Arnoldi method. However, Algorithm 5.1 can converge to the desired smallest positive eigenvalue as shown in Table 2(a). In the cases $\varepsilon = 3.0$ and 2.0 [Figure 4(b) and (c)], there are, respectively, no and two reciprocals of the positive eigenvalues which are larger than the absolute values of the reciprocals of the other complex eigenvalues. Algorithm

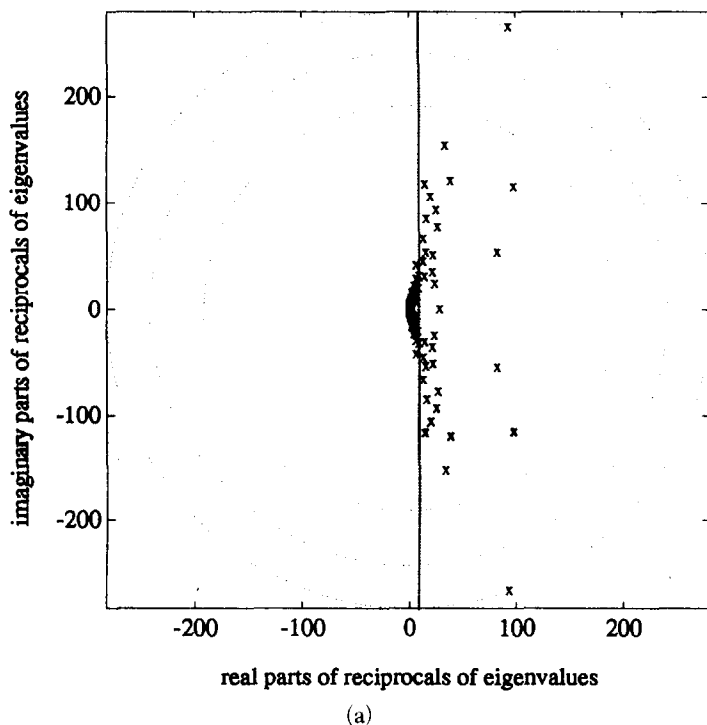


FIG. 4. Reciprocals of the eigenvalues: (a) $\varepsilon = 5.0$, (b) $\varepsilon = 3.0$, (c) $\varepsilon = 2.0$, (d) $\varepsilon = 0.8$.

5.1 can converge to two and three desired positive eigenvalues as shown in Table 2(b) and (c), respectively. If the reciprocals of the positive eigenvalues which are surrounded by the reciprocals of the complex eigenvalues are larger than $1/\gamma_*$ [see (5.1)], then these positive eigenvalues can be found by Algorithm 5.1. In the case $\varepsilon = 0.8$ [Figure 4(d)], Algorithm 5.1 can converge to five positive eigenvalues. The numerical result is shown in Table 2(d). The accuracy of the convergent eigenvalues is at least 12 significant digits.

REMARK. For the quadratic eigenvalue problem (1.1), Algorithm 5.1 computes a few of the smallest positive eigenvalues until the convergent values lie outside of the interval $[0, \gamma_*]$. This value γ_* may be very close to the convergent positive eigenvalues; see Figure 4(c). The values of γ_* are decreasing, and the rate of decrease becomes slow as the number of convergent eigenvalues is increases. Since $\gamma_*^{(j)}$ is the smallest nonnegative

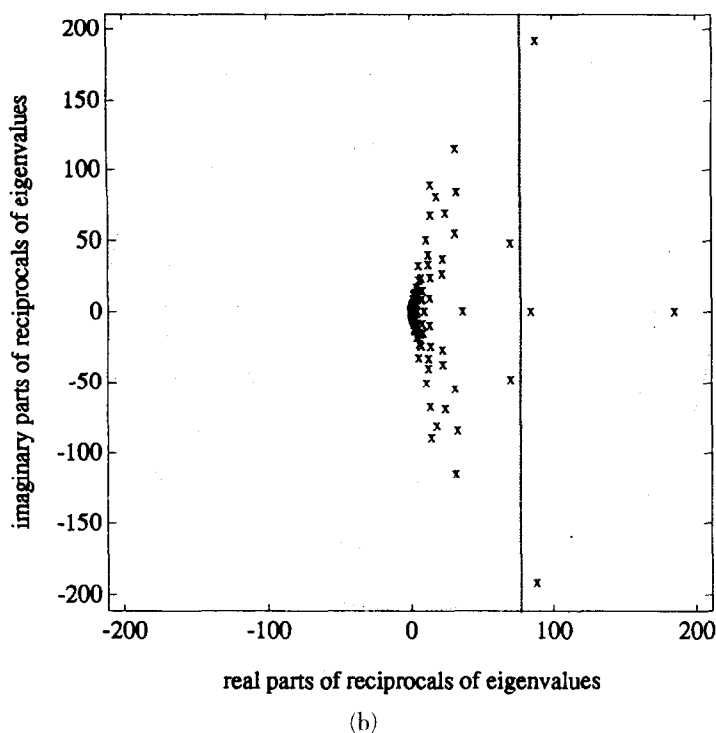


FIG. 4. Continued.

eigenvalue of the pair $(Y_j^T B Y_j, -Y_j^T C Y_j)$ for $j = 1, \dots, m$, where m is the total number of convergent eigenvalues, and the eigenvalues of $(Y_j^T B Y_j, -Y_j^T C Y_j)$, for $j = 1, \dots, m$, are interlaced by the eigenvalues of $(Y_m^T B Y_m, -Y_m^T C Y_m)$, the rate of decrease of $\{\gamma_*^{(j)}\}$ becomes slow as j increases from 1 to m . For typical numerical results one can refer to Table 2(c) and (d).

6. CONCLUSIONS

In this paper, we propose an efficient and reliable algorithm to compute a few of the smallest positive eigenvalues of a large sparse quadratic eigenvalue problem. This method is quite different from the previous methods [7, 14, 16, 21, 22, 23, 24, 25]. Although our algorithm sometimes requires more computational time than the other methods, it guarantees convergence to the

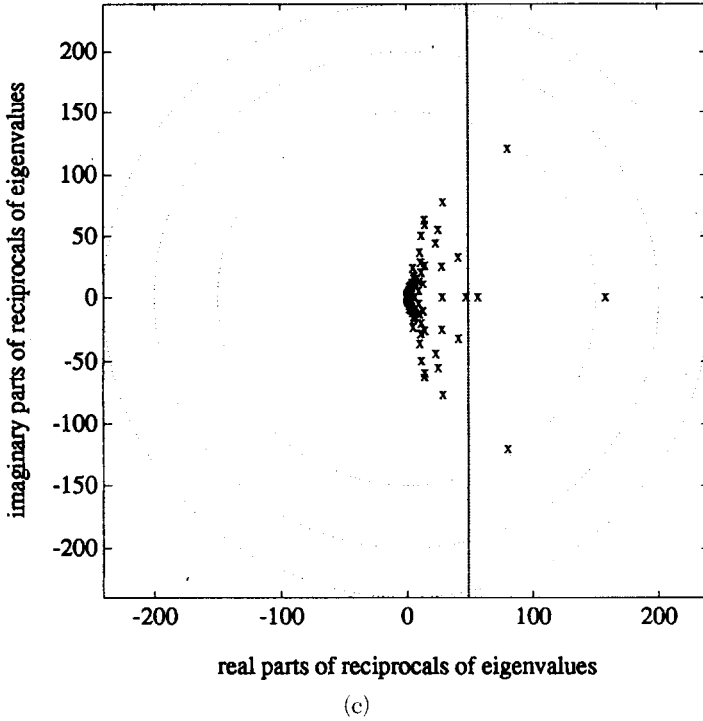


FIG. 4. Continued.

smallest positive eigenvalue even if the reciprocal of this eigenvalue is surrounded by the reciprocals of many complex eigenvalues. In general, at least the basic iteration can converge to this smallest positive eigenvalue. The slow convergence can be accelerated by the tangent-Newton iterations with quadratic convergence rate. The stopping criteria in (5.1), (5.2), and (5.3) of Algorithm 5.1 are reasonable and acceptable.

If the condition (5.1) fails, then the basic iteration can be divergent (as shown in Figure 2). If the condition (5.2) is not satisfied, then the computed eigenvectors can be linearly dependent. This violates the assumption of Theorem 3.4. If (5.3) fails, then the matrix C in the (SP) problem becomes indefinite. The decreasing property of the eigenvalue curve $\beta(\lambda)$ is lost. Hence, Algorithm 5.1 cannot break down in an “unlucky” situation. In comparison with the unsymmetric Lanczos method for solving the quadratic eigenvalue problem, our algorithm avoids computing complex eigenvalues and suffering undetected growth in certain directions of Lanczos vectors [20]. Furthermore, Algorithm 5.1 can be regarded as a global convergence method

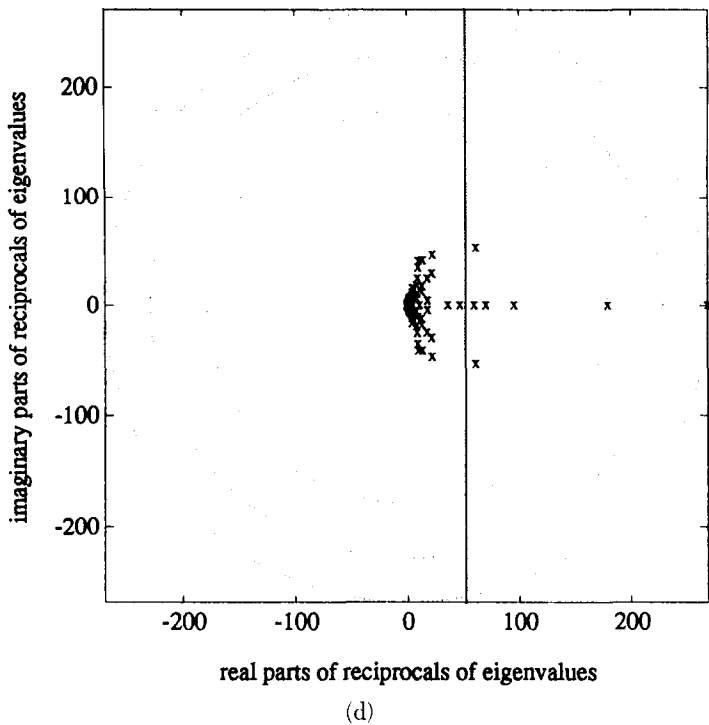


FIG. 4. Continued.

TABLE 2
(a) $n = 100, \varepsilon = 5.0$

No.	Step	Lanczos no.	Rel. Error	Residual	γ_*
1	13	18,20,27,29,30,27,29, 31,32,35,34,33,34	$1.0059\text{E} - 14$	$4.5858\text{E} - 11$	$1.0478\text{E} - 01$
(b) $n = 100, \varepsilon = 3.0$					
1	5	18,19,21,21,21	$6.5664\text{E} - 13$	$3.3072\text{E} - 12$	$1.8384\text{E} - 02$
2	6	22,22,25,26,29,26	$4.1037\text{E} - 12$	$6.1010\text{E} - 11$	$1.2970\text{E} - 02$
(c) $n = 100, \varepsilon = 2.0$					
1	5	18,18,18,18,19	$3.7157\text{E} - 13$	$1.1755\text{E} - 12$	$2.5462\text{E} - 02$
2	5	19,19,20,19,20	$1.2024\text{E} - 12$	$3.4572\text{E} - 12$	$2.0975\text{E} - 02$
3	5	23,25,28,28,28	$4.8090\text{E} - 13$	$1.9432\text{E} - 11$	$2.0456\text{E} - 02$
(d) $n = 100, \varepsilon = 0.8$					
1	4	18,18,17,18	$6.0700\text{E} - 13$	$8.2904\text{E} - 13$	$4.3070\text{E} - 02$
2	4	19,19,18,19	$7.3935\text{E} - 13$	$7.2123\text{E} - 13$	$3.9345\text{E} - 02$
3	6	20,22,22,23,18,13	$6.2932\text{E} - 13$	$3.3419\text{E} - 13$	$3.3652\text{E} - 02$
4	6	22,23,24,24,24,24	$2.1175\text{E} - 13$	$2.1877\text{E} - 12$	$2.4244\text{E} - 02$
5	5	23,25,24,24,24	$2.4721\text{E} - 12$	$8.0258\text{E} - 12$	$1.9047\text{E} - 02$

to compute some desired eigenvalues. It is different from the Newton-type method for solving λ -matrix problems [16, 22, 23], which has only local convergence. It is also worth mentioning that the nonequivalence deflation is more reliable than the implicit successive deflation [23] when two desired eigenvectors are not orthogonal. Besides, the nonequivalence deflation technique preserves the decreasing property of eigenvalue curves, so that our algorithm ensures convergence.

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